

Errors and uncertainties in chemistry internal assessment

The consideration and appreciation of the significance of the concepts of errors and uncertainties helps to develop skills of inquiry and thinking that are not only relevant to the group 4 experimental sciences. The evaluation of the reliability of the data upon which conclusions can be drawn is at the heart of a wider scientific method that IB students consider in other areas such as group 3 individuals and societies, and theory of knowledge. They then may apply this in their subsequent educational, professional and personal lives.

Errors and uncertainties are addressed in “Topic 11: Measurement and data processing” of the subject guide and this topic can be very effectively treated through the practical scheme of work.

The treatment of errors and uncertainties is directly relevant in the internal assessment criteria of:

- data collection and processing, aspects 1 and 3 (recording raw data and presenting processed data)
- conclusion and evaluation, aspects 1, 2 and 3 (concluding, evaluating procedure(s), and improving the investigation).

Expectations at standard level and higher level

The expectations with respect to errors and uncertainties in internal assessment are the same for both standard and higher level students and are supported by topic 11 of the subject guide.

Within internal assessment students should be able to do the following:

- make a quantitative record of uncertainty range (\pm) (data collection and processing: aspect 1)
- state the results of calculations to the appropriate number of significant figures. The number of significant figures in any answer should reflect the number of significant figures in the given data (data collection and processing: aspect 3).
- propagate uncertainties through a calculation so as to determine the uncertainties in calculated results and to state them as absolute and/or percentage uncertainties (this applies to both higher and standard level students). Only a simple treatment is required. For functions such as addition and subtraction absolute uncertainties can be added. For multiplication, division and powers, percentage uncertainties can be added. If one uncertainty is much larger than others, the approximate uncertainty in the calculated result can be taken as due to that quantity alone (data collection and processing: aspect 3).
- determine from graphs physical quantities (with units) by measuring and interpreting a slope (gradient) or intercept. When constructing graphs from experimental data, students should make an appropriate choice of axes and scale, and the plotting of points should be clear and accurate. (Millimetre square graph paper or software is appropriate. Quantitative measurements should not be made from sketch graphs.) The uncertainty requirement can be satisfied by drawing best-fit curves or straight lines through data points on the graph (data collection and processing: aspect 3). (Note: Chemistry students at SL and HL are not expected to construct uncertainty bars on their graphs and may achieve “complete” for aspect 3 of data collection and processing without them. However, students, probably those who also study IB physics, often construct error bars and there is no requirement to discourage them from doing so.)
- justify their conclusion by discussing whether systematic errors or further random errors were encountered. The direction of any systematic errors should be appreciated. The percentage error should be compared with the total estimated random error as derived from the propagation of uncertainties (conclusion and evaluation: aspect 1).
- comment about the precision and accuracy of the measurements when evaluating their procedure (conclusion and evaluation: aspect 2)
- suggest how the effects of random uncertainties may be reduced and systematic errors be eliminated. Students should be aware that random, but not systematic, errors are reduced by repeating readings (conclusion and evaluation: aspect 3).

Explaining terms and concepts

(a) Random and systematic error

Systematic errors arise from a problem in the experimental set-up that results in the measured values always deviating from the “true” value in the same direction, that is, always higher or always lower. Examples of causes of systematic error are miscalibration of a measuring device or poor insulation in calorimetry experiments.

Random errors arise from the imprecision of measurements and can lead to readings being above or below the “true” value. Random errors can be reduced with the use of more precise measuring equipment or its effect minimized through repeat measurements so that the random errors cancel out.

(b) Accuracy and precision

Accuracy is how close a measured value is to the correct value, whereas **precision** indicates how many significant figures there are in a measurement. For example, a mercury thermometer could measure the normal boiling temperature of water as 99.5° C ($\pm 0.5^\circ$ C) whereas a data probe recorded it as 98.15° C ($\pm 0.05^\circ$ C). In this case the mercury thermometer is more accurate whereas the data probe is more precise. Students should appreciate the difference between the two concepts (topic 11.1.2).

(c) Uncertainties in raw data

When numerical data is collected, values cannot be determined exactly, regardless of the nature of the scale or the instrument. If the mass of an object is determined with a digital balance reading to 0.1 g, the actual value lies in a range above and below the reading. This range is the uncertainty of the measurement. If the same object is measured on a balance reading to 0.001 g, the uncertainty is reduced, but it can never be completely eliminated. When recording raw data, estimated uncertainties should be indicated for all measurements.

There are different conventions for recording **uncertainties in raw data**.

- The simplest is the least count, which simply reflects the smallest division of the scale, for example ± 0.01 g on a top pan balance.
- The instrument limit of error: this is usually no greater than the least count and is often a fraction of the least count value. For example, a burette is often read to half of the least count division. This would mean that a burette value of 34.1 cm³ becomes 34.10 cm³ (± 0.05 cm³). Note that the volume value is now cited to one extra decimal place so as to be consistent with the uncertainty.
- The estimated uncertainty takes into account the concepts of least count and instrument limit of error but also, where relevant, higher levels of uncertainty as indicated by an instrument manufacturer, or qualitative considerations such as parallax problems in reading a burette scale, reaction time in starting and stopping a timer, random fluctuation in a voltmeter read-out, or difficulties in knowing just when a colour change has been completed in a rate experiment or titration. Students should do their best to quantify these observations into the estimated uncertainty.

In chemistry internal assessment it is not specified which protocol is preferred and a moderator will support a teacher when it is clear that recording uncertainties has been required and the uncertainties recorded are of a sensible and consistent magnitude.

(d) Propagating errors

Random errors (uncertainties) in raw data feed through a calculation to give an error in the final calculated result. There is a range of protocols for **propagating errors**. A simple protocol is as follows:

1. When **adding or subtracting** quantities, then the **absolute uncertainties are added**.

For example, if the initial and final burette readings in a titration each have an uncertainty of ± 0.05 cm³ then the propagated uncertainty for the total volume is $(\pm 0.05 \text{ cm}^3) + (\pm 0.05 \text{ cm}^3) = (\pm 0.10 \text{ cm}^3)$.

2. When **multiplying or dividing quantities**, then the **percent (or fractional) uncertainties are added**.

For example,

molarity of NaOH(aq) = 1.00 M (± 0.05 M) percent uncertainty = $[0.05/1.00] \times 100 = 5\%$

volume of NaOH(aq) = 10.00 cm³ (± 0.10 cm³) percent uncertainty = $[0.10/10.00] \times 100 = 1\%$

Therefore, calculated moles of NaOH in solution = $1.00 \times [10.00/1000] = 0.0100$ moles ($\pm 6\%$)

The student may convert the calculated total percent uncertainty back into an absolute error or leave it as a percentage.

Note: A common protocol is that the final total percent uncertainty should be cited to no more than one significant figure if it is greater than or equal to 2% and to no more than two significant figures if it is less than 2%.

There are other protocols for combining uncertainties such as “root sum of square” calculations. These are not required in IB chemistry but are acceptable if presented by a student.

(e) Repeated measurements

Repeated measurements can lead to an average value for a calculated quantity. The final answer could be given to the propagated error of the component values in the average.

For example,

$$\Delta H_{\text{mean}} = 102 \text{ kJ mol}^{-1} (\pm 10\%)$$

$$\Delta H_{\text{mean}} = [+100 \text{ kJ mol}^{-1} (\pm 10\%) + 110 \text{ kJ mol}^{-1} (\pm 10\%) + 108 \text{ kJ mol}^{-1} (\pm 10\%)] / 3$$

This is more appropriate than adding the percent errors to generate 30%, since that would be completely contrary to the purpose of repeating measurements. A more rigorous method for treating repeated measurements is to calculate standard deviations and standard errors (the standard deviation divided by the square root of the number of trials). These statistical techniques are more appropriate to large-scale studies with many calculated results to average. This is not common in IB chemistry and is therefore not a requirement in chemistry internal assessment.

Interpreting the relevant assessment criteria

Data collection and processing: Aspect 1 (recording raw data)

Sample extracts of typical student work from an experiment on volumetric analysis in acid-base titration are shown in tables 1–3.

Table 1: DCP aspect 1 = “partial”

Table 1

a. Titration of standard NaOH against vinegar

Final volume / cm ³	42.5	41.5
Initial volume / cm ³	2.5	1
Volume of base required / cm ³	40.0	40.5
Colour of solution at end point	light pink	dark pink

Some appropriate raw data is recorded but there are no uncertainties and the number of decimal places is inconsistent. Either of these factors reduces the level of achievement for aspect 1 of data collection and processing to **partial/1**.

Table 2: DCP aspect 1 = “partial”

Table 2

b. Titration of standard HCl against NaOH

	Run 1	Run 2	Run 3
Initial volume / cm ³ (±0.1 cm ³)	0.0	2.7	1.0
Final volume / cm ³ (±0.1 cm ³)	42.2	42.7	41.5
Volume of base required / cm ³ (±0.2 cm ³)	42.2	40.0	40.5

Some appropriate raw data is recorded with units and uncertainties. However, relevant qualitative observations were not recorded and the level of achievement for aspect 1 of data collection and processing is **partial/1**.

Table 3: DCP aspect 1 = “complete”

Table 3

c. Titration of 5.00 cm³ vinegar against the standardized NaOH

	Trial	Trial	Trial
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	1	2	3
Initial volume / cm ³ (± 0.05 cm ³)	1.00	2.55	0.00
Final volume / cm ³ (± 0.05 cm ³)	42.50	43.25	40.50
Total volume of base required / cm ³ (± 0.1 cm ³)	41.5	40.7	40.5

Colours of solutions: acid, base and phenolphthalein indicator were all colourless. At the end point, the rough trial was dark pink. The other two trials were only slightly pink at the end point.

The student records appropriate qualitative and quantitative raw data, including units and uncertainties. The level of achievement for aspect 1 of data collection and processing is **complete/2**.

The following examples of data collection and processing (see tables 4–6) are from a gas law experiment.

Table 4: DCP aspect 1 = “complete”

Table 4

Temperature T / °C ± 0.2 °C	Height of column h / mm ± 0.5 mm
10.5	58.0
20.3	60.5
30.0	61.0
39.9	64.0
50.1	64.5
60.2	67.5
70.7	68.0
80.8	71.0
90.0	71.5

In table 4, the student designed the data table and correctly recorded the raw data, including units and uncertainties. The level of achievement for aspect 1 of data collection and processing is **complete/2**.

Table 5: DCP aspect 1 = “partial”

Table 5

Temperature (T)	Height of column (h)
10.5	58.0
20.3	60.5
30.0	61.0
39.9	64.0
50.1	64.5
60.2	67.5
70.7	68.0
80.8	71.0
90.0	71.5

In table 5, units and uncertainties are not included. The level of achievement for aspect 1 of data collection and processing is **partial/1**.

Table 6: DCP aspect 1 = “partial”

Table 6

Temperature	Height of column
10.5	58
20.3	60.5
30	61
39.9	64
50	64.5
60.2	67.5
70.7	68
80.8	71
90	71.5

In table 6, units and uncertainties are not included, and the data is recorded in an inconsistent manner. Significant digits are not appreciated. The level of achievement for aspect 1 of data collection and processing is **partial/1**.

Note: In investigations where a very large amount of data is recorded (probably by a data logger), it may be more appropriate to present the data as a graph. The uncertainties should be recorded on the axis labels and any qualitative observations recorded as annotations on or below the graph.

Data collection and processing: Aspect 3 (presenting processed data)

Figures 1 and 2 show graphs of the gas law data from table 4.

Figures 1 and 2: DCP aspect 3 = “complete”

Figure 1

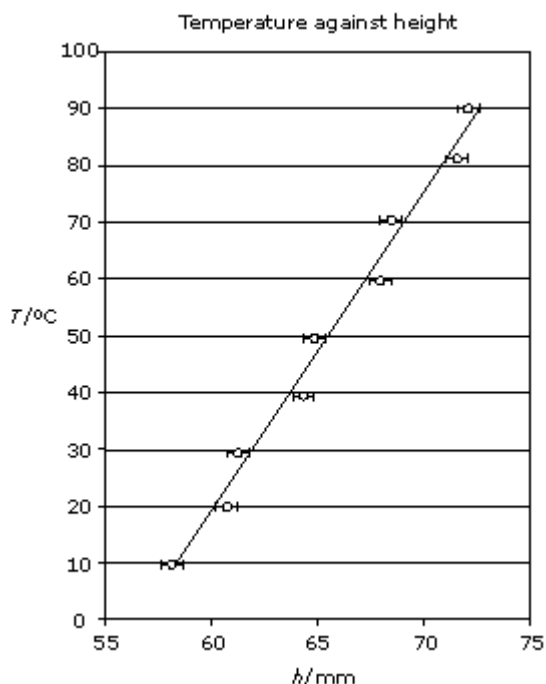


Figure 2

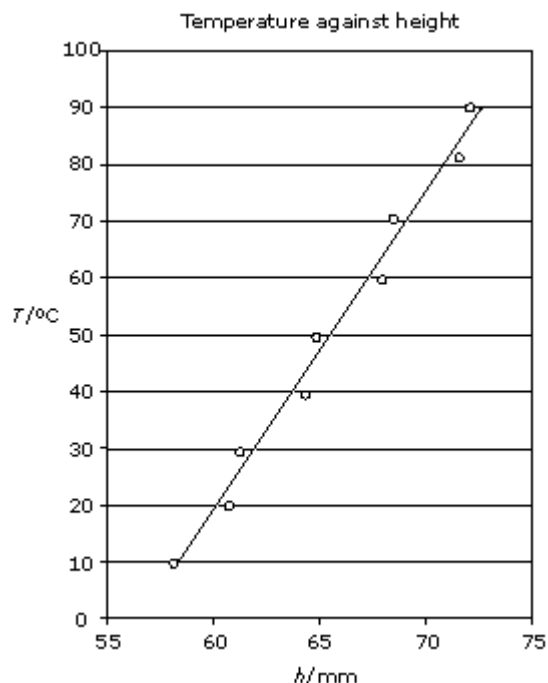
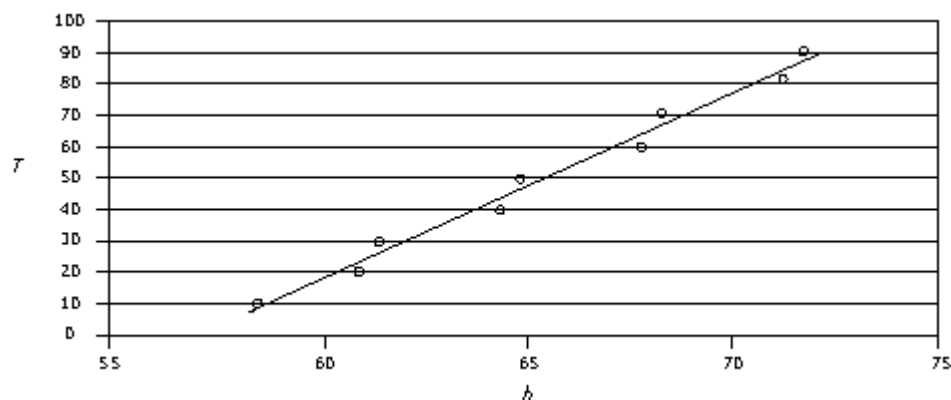


Figure 1 is a graph of the gas law data showing the significant uncertainty. The computer drew the uncertainty bars based on the student entering the correct information, which in this case was 0.5 mm for each value. Figure 2 does not show the uncertainty bars. In chemistry, students are **not** expected to construct uncertainty bars. In both graphs the title is given (although it should be more explicit), and the student has labelled the axes and included units. The level of achievement for aspect 3 of data collection and processing for both graphs is **complete/2**.

Figure 3: DCP aspect 3 = "partial"

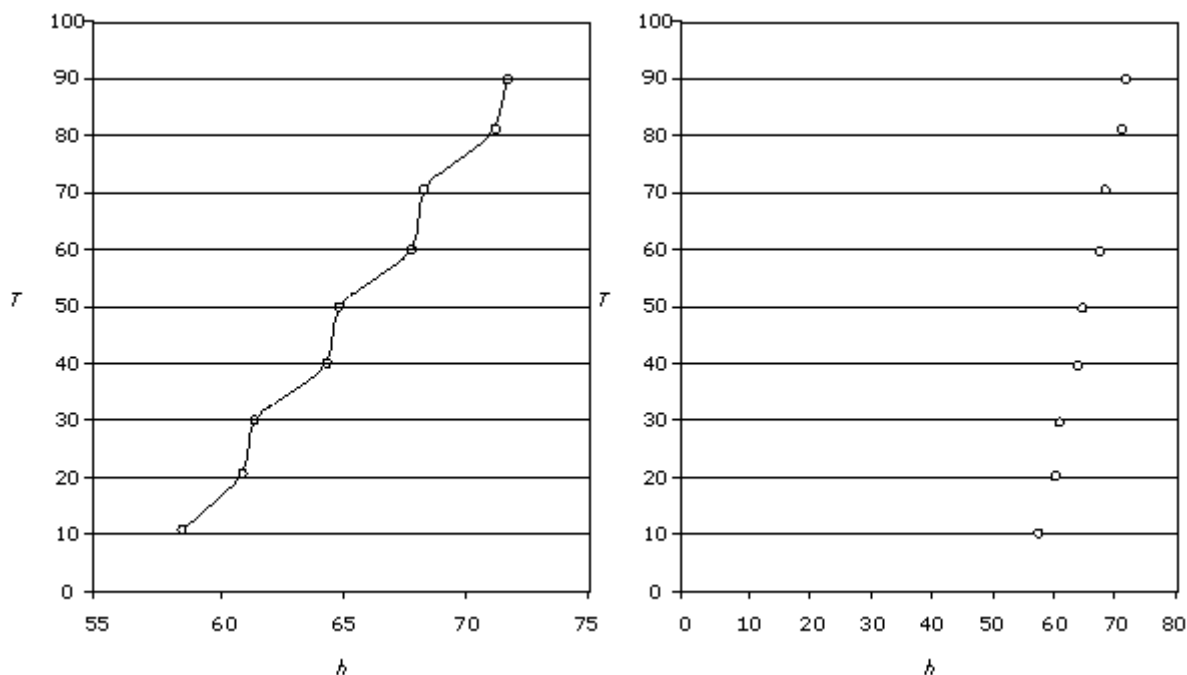
Figure 3



In figure 3, the student does not include a title for the graph, and the units are missing. The level of achievement for aspect 3 of data collection and processing is **partial/1**.

Figure 4: DCP aspect 3 = "not at all"

Figure 4



In the examples shown in figure 4, the first student has failed to draw a best-fit line graph and the second has drawn no line at all. The units and the titles of the graphs are missing. In the second graph, poor use is made of the x-axis scale/ The level of achievement for aspect 3 of data collection and processing for both graphs is **not at all/0**.

Conclusion and evaluation: Aspects 1, 2 and 3 (concluding, evaluating procedure and improving the investigation)

When attempting to measure an already known and accepted value of a physical quantity, such as the charge of an electron, the melting point of a substance, or the value of the ideal gas constant, students can make two types of comments:

1. **The error in the measurement can be expressed by comparing the experimental value with the textbook or literature value.**

Perhaps a student measured the value of the ideal gas constant $R = 8.11 \text{ kPa dm}^3 \text{ mol}^{-1} \text{ K}^{-1}$, and the accepted value is $8.314 \text{ kPa dm}^3 \text{ mol}^{-1} \text{ K}^{-1}$. The error (a measure of accuracy, not precision) is 2.45% of the accepted value. This sounds good, but if, in fact, the experimental uncertainty is only 2%, random errors alone cannot explain the difference, and some systematic error(s) must be present.

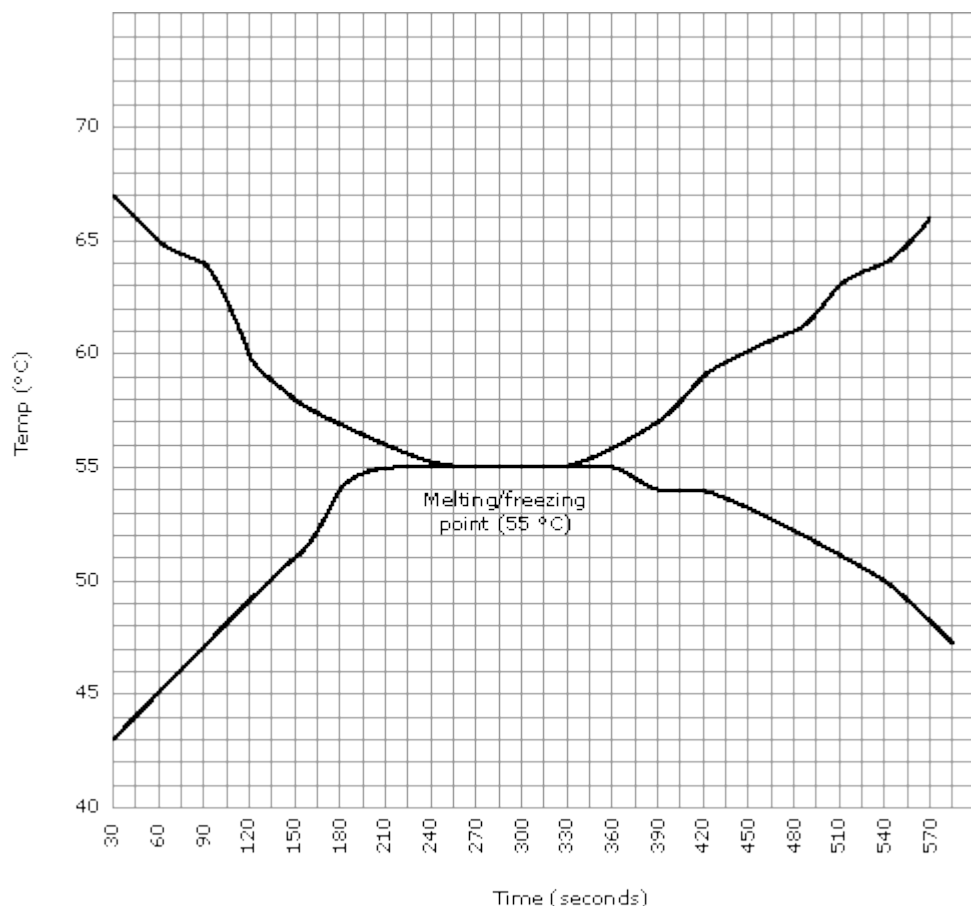
2. **The experimental results fail to meet the accepted value** (a more relevant comment).

The experimental range does not include the accepted value. The experimental value has an uncertainty of only 2%. A critical student would appreciate that they must have missed something here. There must be more uncertainty and/or errors than acknowledged.

In addition to the above two types of comment, students may also comment on errors in the assumptions of the theory being tested, and errors in the method and equipment being used. Two typical examples of student work are given in figures 5 and 6.

Figure 5: CE aspect 1 = "partial", aspect 2 = "not at all"

Figure 5

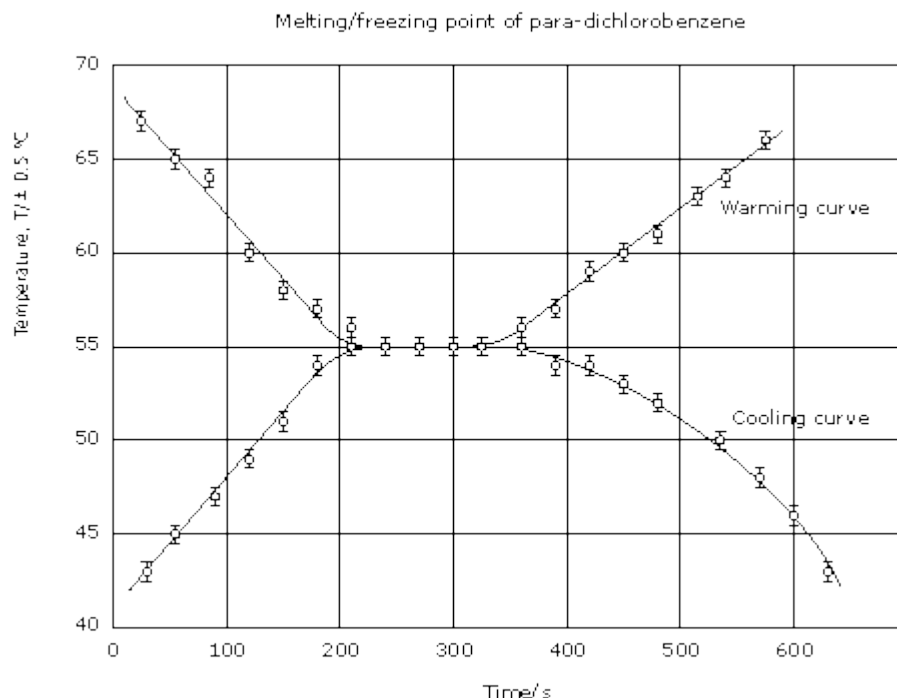


Conclusion and evaluation: Intermolecular bonds are being broken and formed which consumes energy. There is a definite correlation between the melting point and the freezing point of a substance. If good data is collected, the melting point should be the same as the freezing point. A substance should melt, go from solid to liquid, at the same temperature that it freezes, goes from liquid to solid. Our experiment proved this is true because, while freezing, the freezing point was found to be 55 °C, and when melting, the melting point was also found to be 55 °C (see graph).

The student states a conclusion that has some validity. No comparison is made with the literature value. There is no evaluation of the procedure and results. The level of achievement for aspect 1 of conclusion and evaluation is **partial/1**. The level of achievement for aspect 2 is **not at all/0**.

Figure 6: CE aspects 1, 2 and 3 = "complete"

Figure 6



Melting point = freezing point = 55.0 ± 0.5 °C

$$\% \text{ uncertainty} = \frac{0.5}{55.0} \times 100 = 0.9\%$$

Conclusion and evaluation: Literature value of melting point of para-dichlorobenzene = 53.1° C (Handbook of Chemistry and Physics).

$$\therefore \% \text{ difference} = \frac{55.0 - 53.1}{53.1} \times 100 = 3.58\%$$

The fact that % difference > % uncertainty means random errors alone cannot explain the difference and some systematic error(s) must be present.

Melting point (or freezing point) is the temperature at which the solid and the liquid are in equilibrium with each other: (s) \rightleftharpoons (l). This is the temperature at which there is no change in kinetic energy (no change in temperature), but a change in potential energy. The value suggests a small degree of systematic error in comparison with the literature value as random errors alone are unable to explain the percentage difference.

Evaluation of procedure and modifications:

1. Duplicate readings were not taken. Other groups of students had % uncertainty > % difference, that is, in their case random errors could explain the % difference, so repeating the investigation is important.
2. How accurate was the thermometer? It should have been calibrated. In order to eliminate any systematic errors due to the use of a particular thermometer, calibration against the boiling point of water (at 1 atmosphere) or better still against a solid of known melting point (close to the melting point of the sample) should be done.
3. The sample in the test tube was not as large as in other groups. Thus the temperature rises/falls were much faster than for other groups. A greater quantity of solid, plus use of a more accurate thermometer (not 0.5°C divisions, but the longer one used by some groups) would have provided more accurate results.

The level of achievement for aspects 1, 2 and 3 of conclusion and evaluation is **complete/2**.